Tris(2-chloroethyl) phosphate 115-96-8 | DTXSID5021411

Model Performance

_			
N	Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.58

Global applicability domain: Inside

Local applicability domain index: 5.07e-01

Confidence level: 4.50e-01

Nearest Neighbors from the Training Set

Image not found

Tris(2-chloroethyl) phosphate

Measured: 1.44 Predicted: 1.58 Image not found

Heptenophos Measured: 2.32

Predicted: 2.25

Image not found

Dichlorvos Measured: 1.43

Predicted: 1.25

Image not found

Propetamphos Measured: 3.82 Predicted: 3.21 Image not found

Sarin

Measured: 0.3 Predicted: 3.86e-01